

# Synthesis, crystal structure determination and photoluminescence properties of a pure anti *trans-trans* phenylenevinylene derivative



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## ABSTRACT

Configurational pure anti *trans-trans* phenylenevinylene derivatives (PVs) with appropriate terminal functional groups are important in several applications, such as in the synthesis of frameworks with homogeneous topology along the structure when precise optoelectronic properties are required, for example in chemical sensors. As a clear approach for obtaining PVs with this characteristic, it was established that a simple solvothermal Heck cross-coupling reaction yields a stereospecific  $2^{1/2}$  PV system, whose photoluminescence properties were examined and the crystal structure showed the desired anti *trans-trans* configuration.

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## 1. Introduction

Oligo and poly-phenylenevinylenes related compounds (PVs) have acquired great importance during the last years, mainly due to their remarkable optoelectronic properties [1–8] and promising and current applications in sensing [9,10], electrochemistry [11–14], energy transfer [15–17], OLEDs [18,19], and recent innovations like luminescent MOFs [20], *inter alia*.

It is well known that optoelectronic properties of most molecules are related to their chemical structure, spatial organization and electronic transference across the orbitals arrangements. In the case of PVs, these particular characteristics can be controlled by means of the synthesis method regarding the stereoselectivity of the chosen reaction [21,22]. Although the most spread synthetic methodologies for PVs are the Wittig [8,23,24] and Gilch [25–27] reactions due to their easiness, simplicity and high yields, these reactions are not stereoselective towards the formation of pure *trans* conjugated molecules, which is the key for obtaining optimal luminescent properties in PVs derivatives [28]. As a solution for this stereoselectivity issue, emerged the Heck cross coupling reaction [29,30] which may guarantee configurationally pure *trans* PV molecules and, even though, the early reports of this protocol do not exhibit good yields for the synthesis of PVs [31], several advances have been achieved regarding to this [32,33].

Additionally to the configuration concern, and taking as example PV oligomers with  $2^{1/2}$  electronic conjugation length, it must be considered the spatial relation between rings A and C in PV derivatives (Figs. 1 and 2). As reported [32], the Heck reaction can yield *anti* or *syn* conformations between these rings as a consequence of the configuration, where the *anti* conformation, combined with the *trans-trans* configuration, ensure the optimal arrangement of  $\pi$ -orbitals for the electronic communication across the PV structure through a completely planar structure (Fig. 1d).

However, it is important to take into account that normally the standard Heck methodology is catalogued as stereoselective and not stereospecific, whereby it would be possible to obtain more than one isomer/conformer as products of the reaction (Fig. 1a–f) [34].

As a continuation to our previous work about this matter, [33,35,36], in this paper we report the stereospecific synthesis of a PV derivative through the Heck cross coupling reaction and the crystal structure determination that elucidates the configuration and spatial relation between the external rings A and C.

## 2. Materials and methods

Commercially available precursors were used as received without further purification and solvents were dried according to standard procedures. Melting points were determined on a Bibby Stuart Scientific SMP10 apparatus.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were taken using a Bruker Avance 400 spectrometer with  $\text{CDCl}_3$  as solvent and internal standard for chemical shifts in ppm. LC–MS analysis were obtained in a Shimadzu LCMS-2010 with

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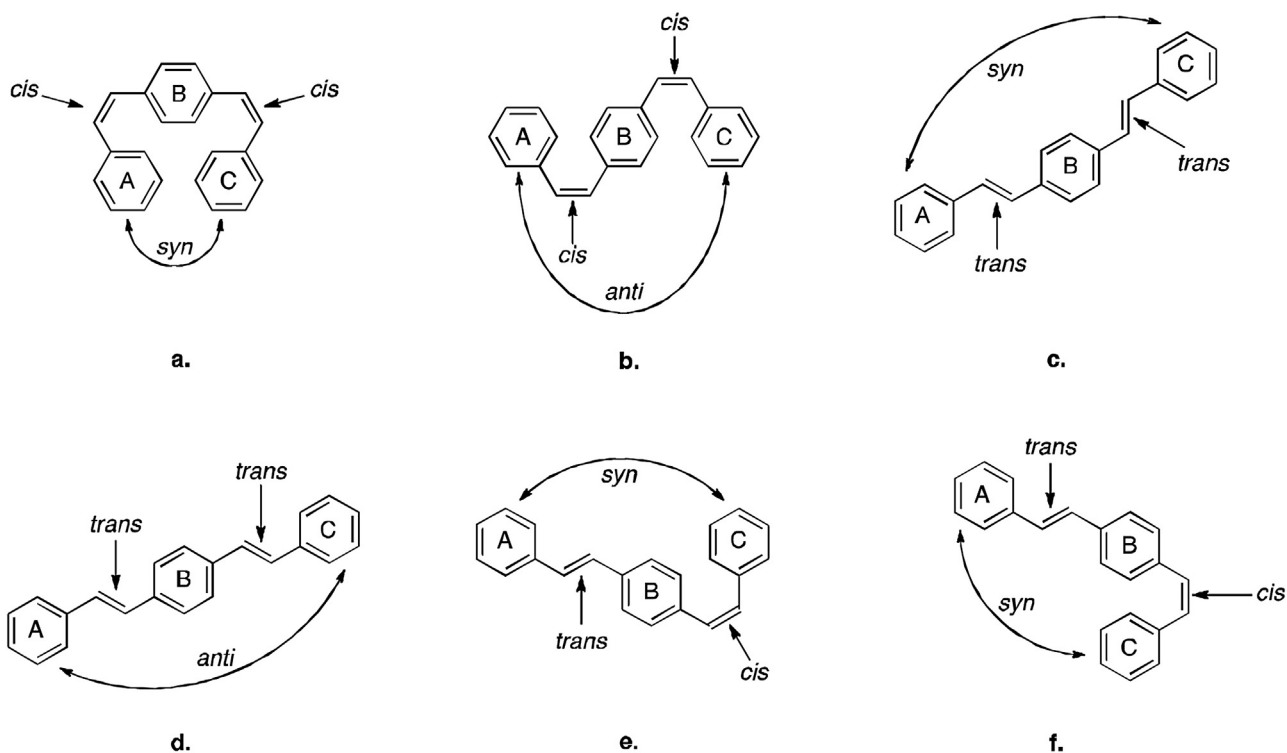


Fig. 1. Configurations and spatial relations of  $2\frac{1}{2}$  length PV molecules.

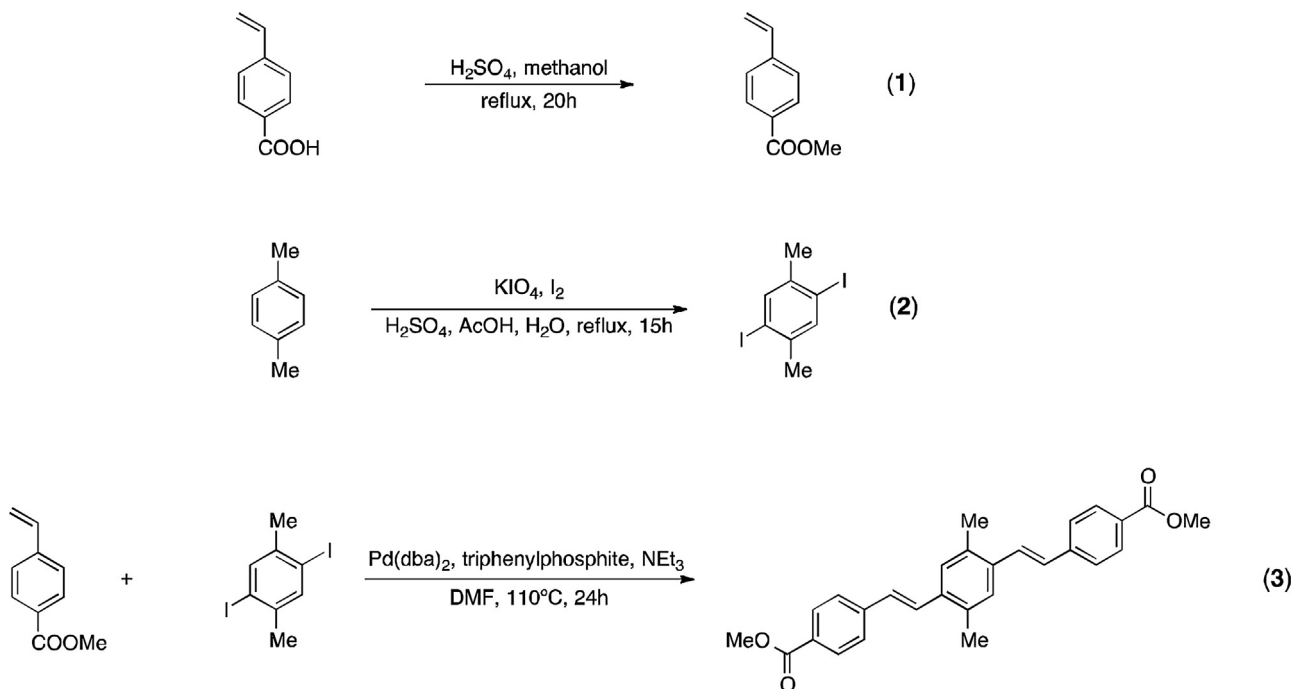


Fig. 2. Synthesis of pure trans PV derivative 3.

electrospray ionization and quadrupole using a Zorbax Bonus – RP column ( $150 \times 2.1$  mm,  $5 \mu\text{m}$ ) and detection at 305 and 350 nm. UV/VIS spectra were measured in a double channel Thermo Scientific Evolution 300 UV/VIS spectrophotometer with xenon lamp based platform. Fluorescence spectra were registered in

DMSO solutions on a PTI QuantaMaster 300 spectrofluorometer with xenon lamp.

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